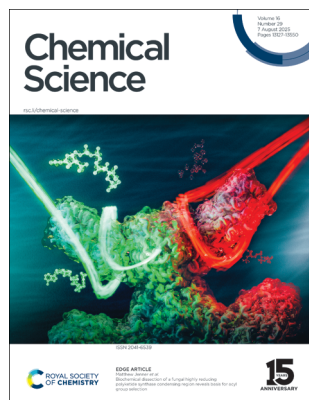


## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 16(29) 13127–13550 (2025)



**Cover**  
See Matthew Jenner *et al.*, pp. 13173–13182. Image reproduced by permission of Matthew Jenner and Munro Passmore from *Chem. Sci.*, 2025, **16**, 13173.



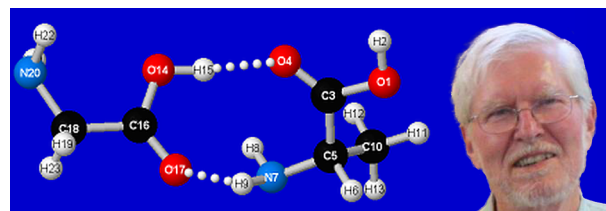
**Inside cover**  
See Kentaro Yonesato, Kosuke Suzuki *et al.*, pp. 13183–13188. Image reproduced by permission of Kosuke Suzuki and Kentaro Yonesato from *Chem. Sci.*, 2025, **16**, 13183.

## PERSPECTIVE

13141

### Personal recollections of a quantum chemist

Frank Weinhold\*

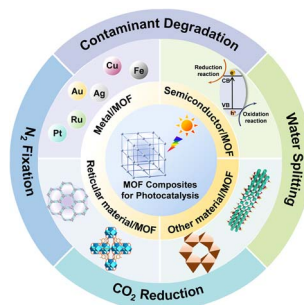


## REVIEW

13149

### Recent advances in MOF composites for photocatalysis

Chenxi Zhang, Yanhong Wu, Dandan Li\* and Hai-Long Jiang\*



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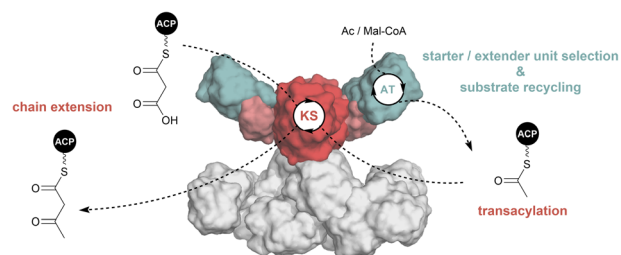
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13173

### Biochemical dissection of a fungal highly reducing polyketide synthase condensing region reveals basis for acyl group selection

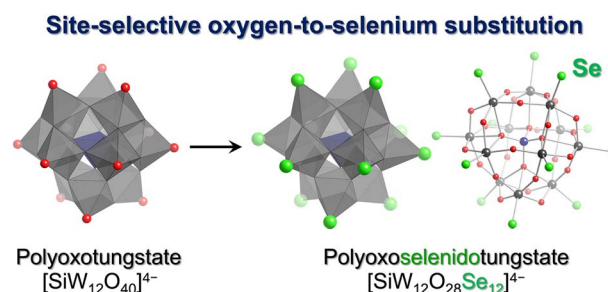
Mia E. Foran, Nazia B. Auckloo, Y. T. Candace Ho, Shaonan Liu, Yang Hai and Matthew Jenner\*



13183

### Synthesis of a Keggin-type polyoxoselenidotungstate via site-selective oxygen-to-selenium substitution

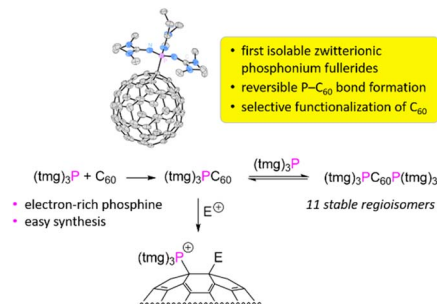
Kentaro Yonesato,\* Yota Watanabe, Magda Pascual-Borràs, R. John Errington, Kazuya Yamaguchi and Kosuke Suzuki\*



13189

### Phosphonium fullerides: isolable zwitterionic adducts of a phosphine with $\text{C}_{60}$

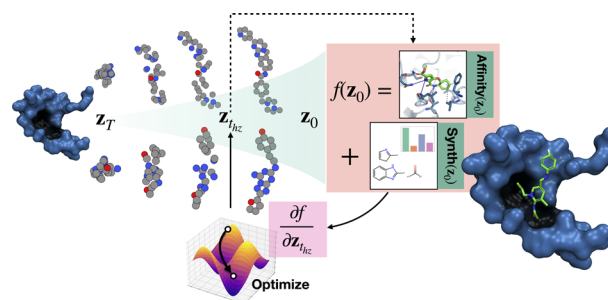
Maike B. Röthel, Jonas H. Franzen, Daniel Leitner, Thomas S. Hofer, Michael Seidl and Fabian Dielmann\*



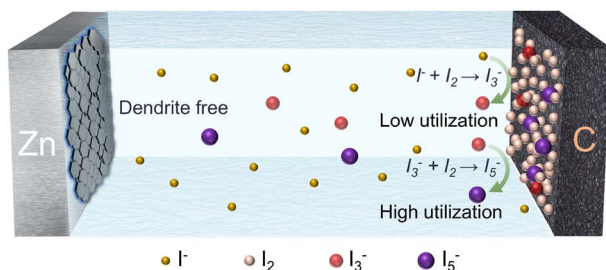
13196

### Guided multi-objective generative AI to enhance structure-based drug design

Amit Kadan,\* Kevin Ryczko,\* Erika Lloyd, Adrian Roitberg and Takeshi Yamazaki\*



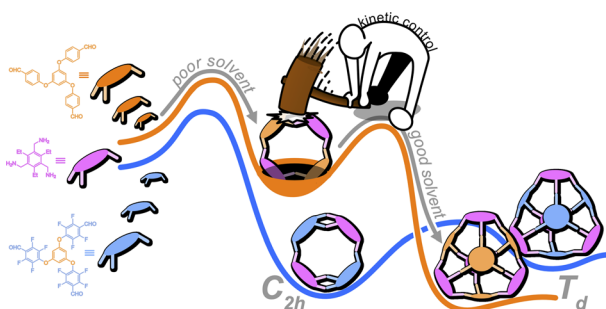
13211



### Iodide-mediated intermediate regulation strategy enables high-capacity and ultra-stable zinc–iodine batteries

Zhijie Xu, Jiaqi Yang, Peng Sun, Yaoyu Chen, Zhengxiao Ji, Xusheng Wang, Min Xu,\* Jinliang Li\* and Likun Pan\*

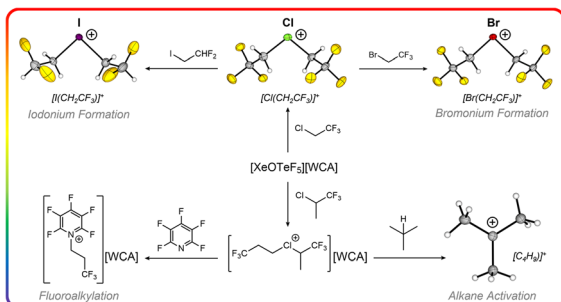
13221



### Structural control of dynamic covalent cages: kinetic vs. thermodynamic assembly and PFAS removal from water

Tobias Pausch, Pablo Martinez Mestre, Fabiola Zapata, Andreas Mix and Bernd M. Schmidt\*

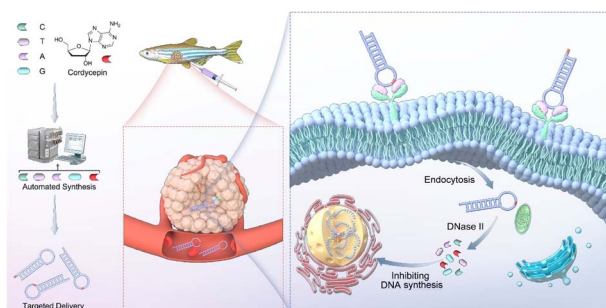
13229



### On the synthesis and structure of reactive halonium ions

Lukas Fischer, Michael H. Lee, Anja Wiesner, Carsten Müller and Sebastian Riedel\*

13235



### Cordycepin: a dual-function molecular element for aptamer engineering with enhanced anticancer activity

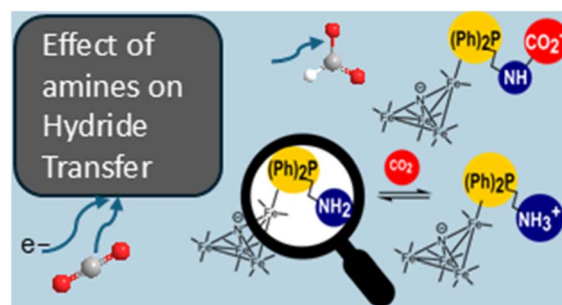
Fei Gao, Li Na, Shuyue Fu, Jinsong Peng, Shipeng He,\* Ruowen Wang\* and Weihong Tan\*



13241

### Amine groups alter product selectivity and rate of catalytic hydride transfer reactions

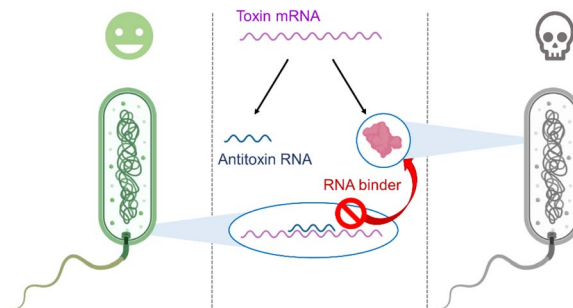
Santanu Pattanayak, Rachel E. Siegel, Yiming Liu, James C. Fettinger and Louise A. Berben\*



13249

### Synthetic RNA ligands as activators of type I toxin–antitoxin systems: a novel antimicrobial strategy targeting *Helicobacter pylori*

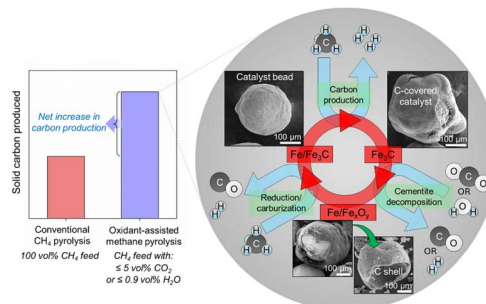
Céline Martin, Marc Panosetti, Eleonora Tesini, Stéphane Azoulay, Anthony Bugaut, Véronique Sinou, Nadia Patino, Audrey Di Giorgio, Fabien Darfeuille\* and Maria Duca\*



13256

### Oxidant-assisted methane pyrolysis

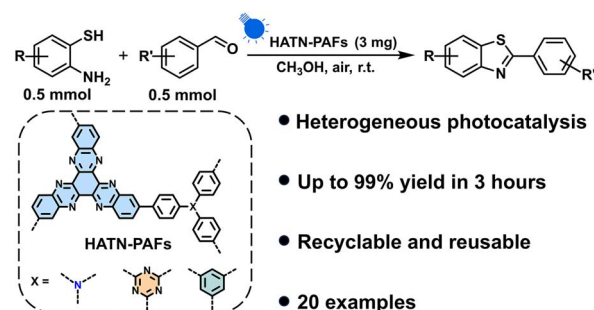
Marco Gigantino, Henry Moise, Vasudev Haribal, Andrew Tong, Jian Ping Shen, Dimitri Saad, Jacob Fishman, Alexander Nelson, Harry Voorhis, Eddie Sun, Adam Brandt, Raghubir Gupta, Arun Majumdar and Matteo Cargnello\*



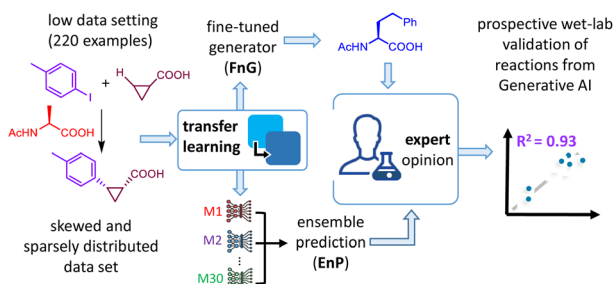
13267

### Optimal photosynthesis of 2-benzothiazoles over hexaazatrinaphthylene-based porous aromatic frameworks

Jingjing Shao, He Wang, Xin Tao\* and Guangshan Zhu



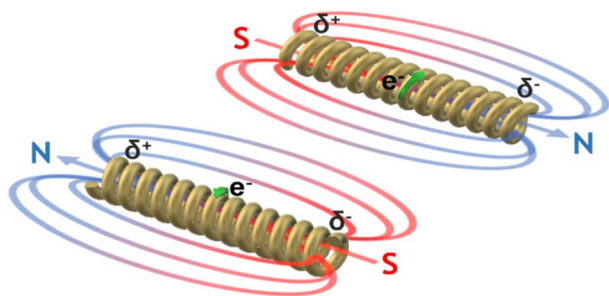
13276



### Molecular Machine Learning Approach to Enantioselective C–H Bond Activation Reactions: From Generative AI to Experimental Validation

Ajnabiul Hoque, Taiwei Chang, Jin-Quan Yu\* and Raghavan B. Sunoj\*

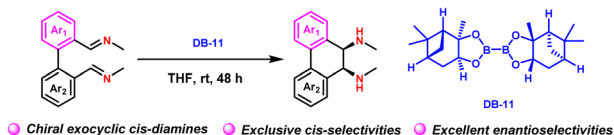
13291



### Exogenous chemically-driven electromagnets

Cara Lozon, Antoine Cornet, Stéphane Reculosa, Patrick Garrigue, Alexander Kuhn and Gerardo Salinas\*

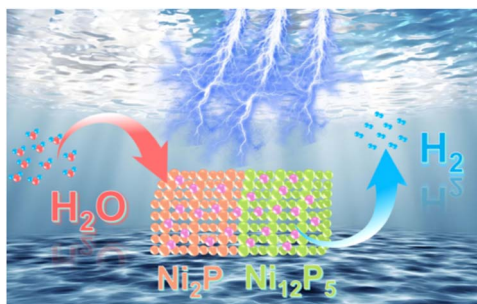
13298



### Asymmetric intramolecular reductive coupling of bisimines templated by chiral ditorons

Tian Chen, Hao-Yang Wang, Ronghua Xu, Guangqing Xu, He Yang,\* Jiangtao Sun,\* Lung Wa Chung\* and Wenjun Tang\*

13306



### Microwave quasi-solid-constructed Ni<sub>2</sub>P–Ni<sub>12</sub>P<sub>5</sub>-supported Os with unique metal–support interaction for anion-exchange membrane seawater electrolysis

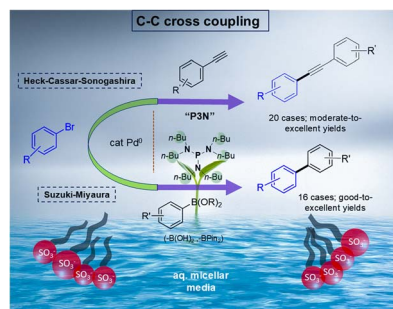
Qing Liu, Xiaowei Fu, Hongdong Li, Jun Xing, Weiping Xiao, Yingxia Zong, Guangying Fu, Jinsong Wang, Qiang Cao, Tianyi Ma,\* Lei Wang\* and Zexing Wu\*



13316

### A new P3N ligand for Pd-catalyzed cross-couplings in water

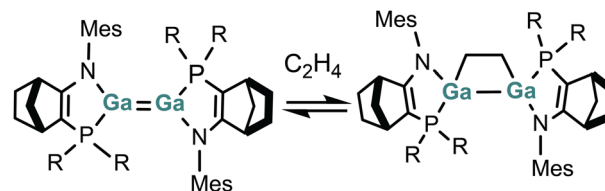
Erfan Oftadeh, Max Baumann, Marco Ortiz, Kirubel Mamo, Eduam Boeira, Esveidy Ocegüera Nava, Monica S. Lopez Lemus, Shili Fang, Donald H. Aue\* and Bruce H. Lipshutz\*



13333

### Reversible addition of ethene to gallium(i) monomers and dimers

Ryan J. Schwamm, Malavika A. Bhide, Gary S. Nichol and Michael J. Cowley\*



Reversible reactivity with ethene

13345

### Intramolecular tension-driven self-recovering mechanochromism in organic microcrystals

Weihan Guo, Hua Zhao, Mingda Wang, Leilei Si, Kaixin Yang, Guomin Xia\* and Hongming Wang\*

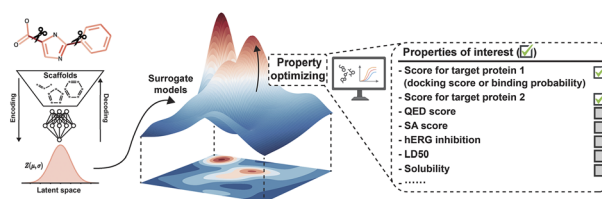
### Self-recovering MCF behavior



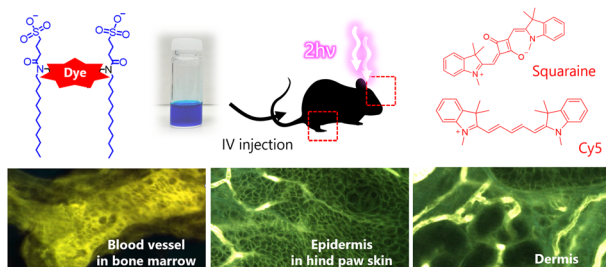
13352

### Multi-objective drug design with a scaffold-aware variational autoencoder

Tiejun Dong, Linlin You\* and Calvin Yu-Chian Chen\*



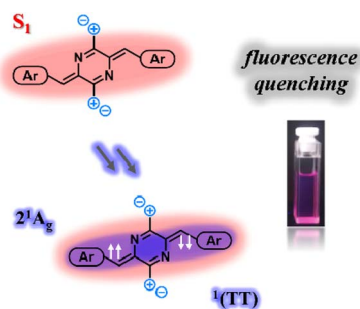
13368



### Bright and water-dispersible membrane probes enable visualization of cellular morphologies and dynamics in light-scattering tissues of living mice

Takumi Uemura, Ryosuke Kawakami, Hitomi Seki, Satoshi Yoshida, Masamoto Murakami, Takeshi Imamura, Hadano Shingo, Shigeru Watanabe and Yosuke Niko\*

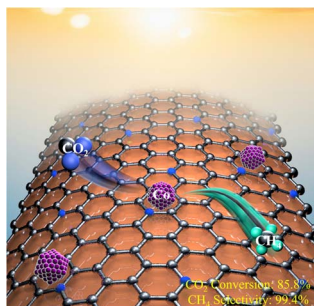
13374



### Side-chain ionization enables ultrafast intramolecular singlet fission in the azaquinodimethane skeleton

Zixiang Wu, Christopher L. Anderson, Teng-Shuo Zhang,\* Yi Liu,\* Hongbing Fu\* and Long Wang\*

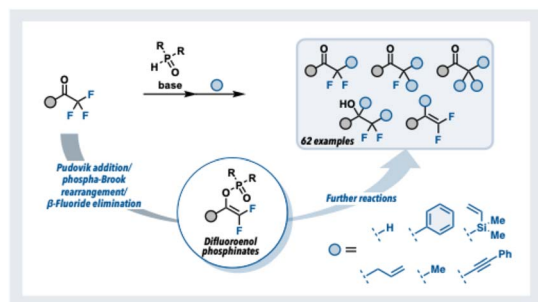
13382



### Controllable construction of cobalt nanoparticles in nitrogen-doped carbon nanotubes for photothermal CO<sub>2</sub> methanation

Zhanghui Xia, Jianxin Zhai, Longfei Lin,\* Xiao Chen, Cheng Xue, Shuaiqiang Jia, Jiapeng Jiao, Mengke Dong, Wanying Han, Xinrui Zheng, Teng Xue, Haihong Wu\* and Buxing Han\*

13390



### Difluoroenol phosphinates as difluoroenolate surrogates: synthesis and applications in defluorination and deoxygenative coupling

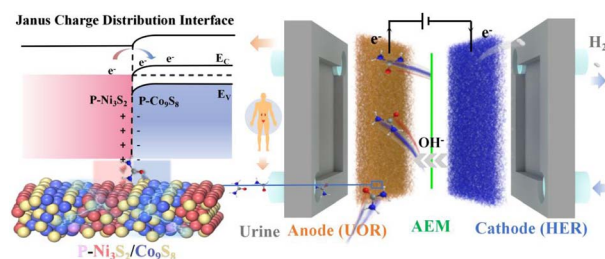
Miki B. Kurosawa, Shuhei Shimoyama, Hiroki Tanaka and Junichiro Yamaguchi\*



13401

### Activating Janus charge distribution on the P-doped $\text{Ni}_3\text{S}_2/\text{Co}_9\text{S}_8$ interface for enhancing charge-matched urea adsorption: boosting high current hydrogen production via coupled urine degradation

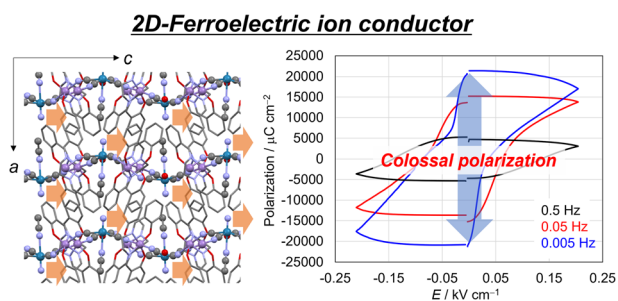
Yan Sun, Xiannan Zhang, Hairui Guo, Wenjiang Li, Huiling Liu\* and Cheng Wang\*



13413

### A ferroelectric proton conductor with colossal polarization induced by in-plane symmetry breaking in a two-dimensional coordination polymer

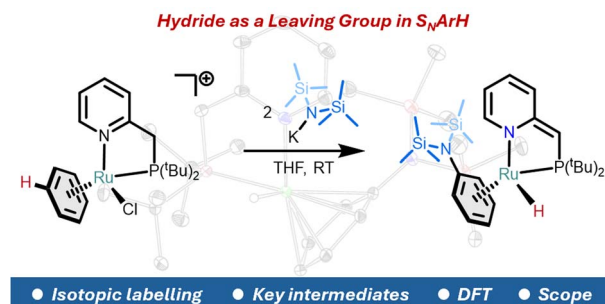
Yanqing Song, Yuta Tsuji, Kunihisa Sugimoto, Takashi Kikuchi, Yuxin Shi, Yusuke Murakami, Kotaro Hiramatsu, Benjamin Le Ouay, Masaaki Ohba\* and Ryo Ohtani\*



13422

### Ruthenium-mediated nucleophilic aromatic substitution of hydrogen in benzene

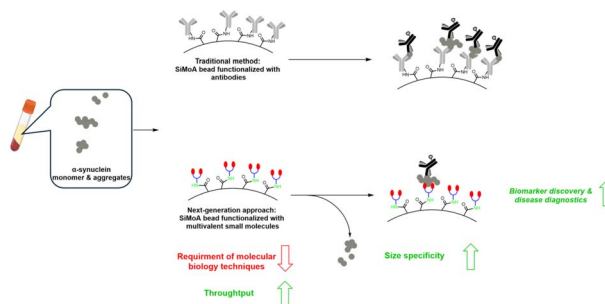
Stanislav Melnikov, Donghun Hwang, Philip Gabbert, Bohyun Park, Martin Lutz, Mu-Hyun Baik\* and Daniël L. J. Broere\*



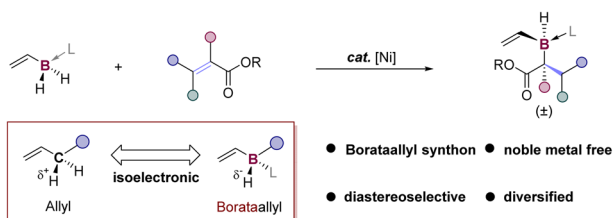
13435

### Detecting alpha-synuclein aggregates with small molecules on single-molecule array

Jeff Y. L. Lam, Timothy S. Chisholm, Hadia Almahli, Elizabeth A. English, Zengjie Xia, Yunzhao Wu, Matthew R. Cheetham,\* Christopher A. Hunter\* and David Klenerman\*



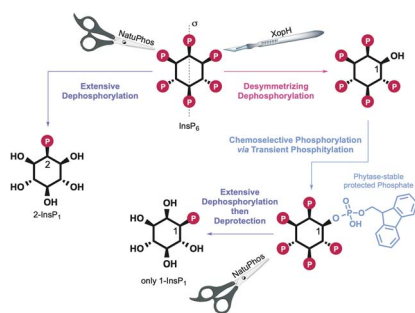
13449



### Nickel-catalyzed diastereoselective hydroboration of acrylates with a vinylborane reagent

Guanwen Hu, Peiqi Zhang, Xinmou Wang, Chunpeng Wan, Yiyi Fu, Wa Hung Leung, Zhenyang Lin\* and Yangjian Quan\*

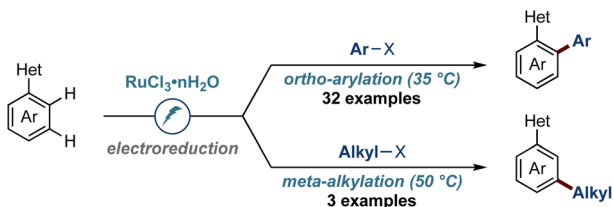
13459



### Stereoselective chemoenzymatic phytate transformations provide access to diverse inositol phosphate derivatives

Georg Markus Häner, Guizhen Liu, Esther Lange, Nikolaus Jork, Klaus Ditrich, Ralf Greiner, Gabriel Schaaf and Henning J. Jessen\*

13468

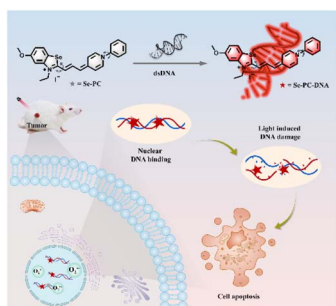


### Electroreductive room-temperature C–H activations with $\text{RuCl}_3 \cdot n\text{H}_2\text{O}$ precatalyst via cathodic ruthenium(III/II) manifold

Takuya Michiyuki, Tristan von Münchow, Zhipeng Lin, Binbin Yuan, João C. A. Oliveira and Lutz Ackermann\*

- Direct utilization of  $\text{RuCl}_3 \cdot n\text{H}_2\text{O}$
- Mild conditions
- Electroreduction
- *ortho*- and *meta*-C–H functionalizations
- Late-stage diversification

13477



### A nuclear targeted type-I photosensitizer for anti-tumor therapy

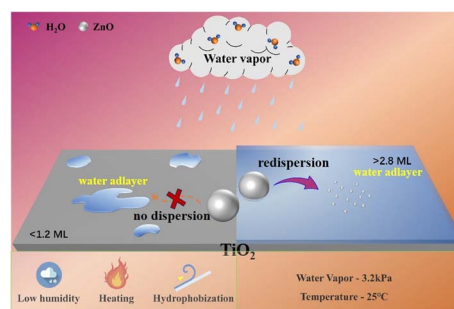
Zipeng Li, Wenkai Liu, Wanying Ma, Changyu Zhang, Jiangli Fan\* and Xiaojun Peng



13486

### Mechanistic insights into spontaneous redispersion of ZnO onto TiO<sub>2</sub> in water-containing environments

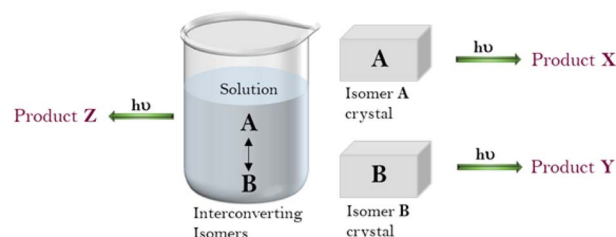
Conghui Liu, Rongtan Li, Xiaohui Feng, Yuting Sun, Yamei Fan, Jiaxin Li and Qiang Fu\*



13496

### Isomer-dependent reactivity in the solid state: topochemical [4 + 4] vs. [4 + 2] cycloaddition reactions

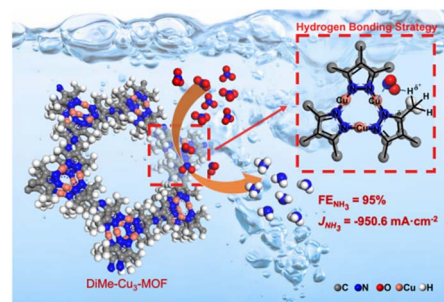
Anu Lal and Kana M. Sureshan\*



13503

### Hydrogen-bond mediated electrocatalytic nitrate reduction to ammonia over metal-organic frameworks with industrial current density

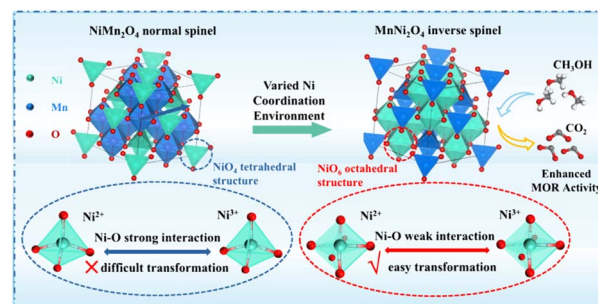
Xiao-Xue Fu, Hui Guo, Duan-Hui Si, Hong-Jing Zhu, Yi-Ying Lan, Yuan-Biao Huang and Rong Cao\*



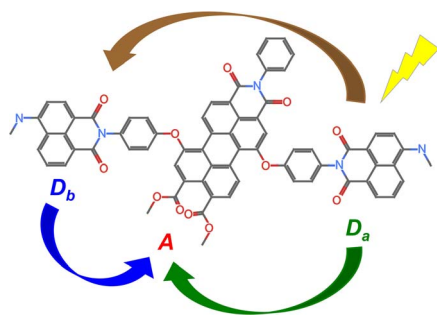
13514

### Insight into Ni active site coordination in nickel-manganese spinels for methanol electrooxidation catalysis

Ruiying Guo, Chunru Liu, Yun Yang,\* Shuli Wang and Ligang Feng\*



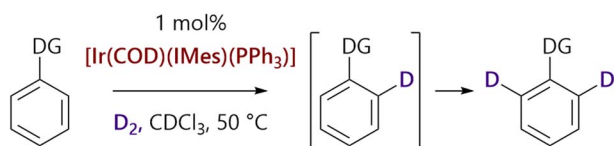
13520



### Simulation of ultrafast transient absorption spectra of a perylene-based light harvesting antenna

Royle Perez-Castillo, Victor M. Freixas, Aliezer Martinez-Mesa, Llinersy Uranga-Piña, Maxim F. Gelin, Sergei Tretiak and Sebastian Fernandez-Alberti\*

13532



### Probing substrate binding and release events in iridium-catalysed hydrogen isotope exchange reactions

Daria S. Timofeeva, William J. Kerr,\* David M. Lindsay\* and David J. Nelson\*

- Mono- versus difunctionalisation in C-H activation
- Categorisation of directing groups based on behaviour
- Key events: associative substrate exchange, C-DG rotation

## CORRECTIONS

13543

### Correction: Pronounced electronic modulation of geometrically-regulated metalloenediyne cyclization

Sarah E. Lindahl, Erin M. Metzger, Chun-Hsing Chen, Maren Pink and Jeffrey M. Zaleski\*

13547

### Correction: Water entropy at the threonine-rich surface of antifreeze and ice-nucleating proteins: small changes make a big difference

Debasis Saha, Rahul Aich, Arnab Mukherjee\* and Biman Jana\*

